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Abraham Model Correlations for Triethylene Glycol Solvent Derived from Infinite Dilution Activity Coefficient, Partition Coefficient and Solubility Data Measured at 298.15 K

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Abstract A gas chromatographic headspace analysis method was used to experimentally determine gas-to-liquid partition coefficients and infinite dilution activity coefficients for 29 liquid organic solutes dissolved in triethylene glycol at 298.15 K. Solubilities were also determined at 298.15 K for 23 crystalline nonelectrolyte organic compounds in triethylene glycol based on spectroscopic absorbance measurements. The experimental results of the headspace chromatographic and spectroscopic solubility measurements were converted to gas-to-triethylene glycol and water-to-triethylene glycol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Expressions were derived for solute transfer into triethylene glycol by combining our measured experimental values with published literature data. Mathematical correlations based on the Abraham model describe the observed partition coefficient and solubility data to within 0.16 $\log_{10}$ units (or less).

Keywords Infinite dilution activity coefficients · Molar solubility ratios · Headspace chromatographic analysis · Partition Coefficients · Solute transfer processes

1 Introduction

Growing environmental concern, combined with increased governmental regulations regarding organic waste disposal, has encouraged the chemical manufacturing sector to explore sustainable approaches in process design. Chemical manufacturers are encouraged to replace hazardous organic solvents with safer chemical alternatives. Replacement of

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